THE GRAPH MATCHING AND QUADRATIC ASSIGNMENT PROBLEMS

by

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A thesis submitted to Johns Hopkins University

in conformity with the requirements for the degree of

Master of Science in Engineering

Baltimore, Maryland

May 2021

Abstract

The graph matching problem seeks to find an alignment between the nodes of two graphs that minimizes the number of edge disagreements. We present a modification to the state-of-the-art graph matching approximation algorithm "FAQ" (Vogelstein, 2015), replacing it's linear sum assignment step with the "Lightspeed Optimal Transport" method of Cuturi (2013). The modification provides a speed improvement by replacing the main computational bottleneck, as well as robustness to stochasticity between graph pairs. The effectiveness of the approach is demonstrated in matching graphs in simulated and real data examples.

Primary Reader and Advisor: Professor Joshua Vogelstein

Secondary Reader: Professor Carey Priebe

Acknowledgments

First, I would like to thank my advisor Joshua Vogelstein for his continued mentorship and support of the work presented, and for allowing me the opportunity to pursue my research interests. This work would not be possible without his guidance. I'd also like to thank Carey Priebe, whose enthusiasm and curiosity for math is contagious. He taught me what it meant to be excited about ones work.

I would like to thank the members of the NeuroData lab for their support. I am indebted to Benjamin Pedigo, who mentored me when I joined the lab, and is always available with a collaborative ear whenever I have an idea or problem. His importance to the work presented is immeasurable.

I'd also like to thank the cohort of graph matching researchers who have provided helpful feedback throughout my research, including Youngser Park, Donniell Fishkind, Vince Lyzinski, and Daniel Sussman. It is a privilege to have the opportunity to work with the leading experts in the field.

Finally, I'd like to thank my friends and family for their support and encouragement. My accomplishments would not be possible without them.

Ali Saad-Eldin

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Chapter 1

Introduction

Graphs are widely used in many fields within the scientific community requiring some degree of pattern recognition, including social networks, computer vision, and neuroscience. In many of these settings, we often work simultaneously with multiple graphs, and want to quantify how they relate to each other. Specifically, we might seek to find a correspondence between the nodes of two graphs such that the connectivity across networks is preserved as best as possible. The Graph Matching Problem consists of finding the bijection between two vertex sets that minimizes the number of edge disagreements. If the two graphs are isomorphic, the graph matching problem should find the exact isomorphism between the two graphs.

The graph matching problem is extremely difficult to solve, and no polynomial-time algorithms exist to solve it in its general form. Indeed, in its most general form, the graph matching problem is equivalent to the famous combinatorial optimization problem, the Quadratic Assignment Problem, which is known to be NP-hard. For this reason, finding accurate, efficient approximation algorithms for the graph matching problem is an active field

of research. There are three main categories of graph matching approximation algorithms: tree search, spectral embedding, and continuous optimization methods.

In this paper, we focus on graph matching via continuous optimization methods. Specifically, we present a modification to the state-of-the art algorithm, *FAQ*, developed by Vogelstein et. al, 2015. The proposed modification, the algorithm *GOAT*, alters the step direction calculation from being a permutation matrix to being a doubly stochastic matrix. Since the step direction is computed during the local optimum search in the relaxed sub problem, it is inefficient to restrict the feasible region. Thus, the modification increases efficiency by decrease running time on larger graphs. Additionally, we will show how GOAT provides performance advantages over FAQ, specifically adding robustness to stochasticity between graph pairs when graph matching.

Chapter 2

Notation and Mathematical Framework

2.1 Quadratic Assignment Problem

Consider two real matrices $A, B \in \mathbb{R}^{n \times n}$. Let $\mathcal{P} = \{P \in \{0,1\}^{n \times n} | P\mathbf{1}_n = \mathbf{1}_n, P^T\mathbf{1}_n = \mathbf{1}_n\}$ be the set of $n \times n$ permutation matrices, where $\mathbf{1}_n$ is the n-dimensional vector of ones. We formally define the Quadratic Assignment Problem (QAP) as the following problem, in matrix notation

$$\begin{aligned} &\min \text{trace}(APB^TP^T) \\ &\text{s.t. } P \epsilon \mathcal{P} \end{aligned} \tag{2.1}$$

The combination of quadratic objective function and non-convex feasible region makes this problem **NP-hard** to solve; no efficient, exact algorithm exists. One could naively solve the problem by finding the objective function value for all permutation matrices in $\mathcal{P}$, however this set is massive, even for small n. For reference, $\mathcal{P}$ is of size $n!$, with more than 10^{157} solutions when $n = 100$. For some of our typical connectomics applications, n is typically

greater than 1,000, meaning that $|\mathcal{P}| > 10^{249}$. We thus seek a method for approximately solving QAP.

Rather than solve the problem over $\mathcal{P}$, we begin by relaxing the feasible to its convex hull, the Birkhoff polytope, also known as the set of doubly stochastic matrices, defined as $\mathcal{D} = \{P \in [0,1]^{n \times n} | P\mathbf{1}_n = \mathbf{1}_n, P^T\mathbf{1}_n = \mathbf{1}_n\}$. We then formally define the relaxed Quadratic Assignment Problem (rQAP) as

$$\begin{aligned} &\min \text{trace}(APB^TP^T) \\ &\text{s.t. } P \epsilon \mathcal{D} \end{aligned} \tag{2.2}$$

We note that even with the relaxation, rQAP is still non-convex due to it's quadratic objective function not having a necessarily positive definite Hessian. Indeed, when A, B are hollow, this Hessian is indefinite. However, the convex feasible region allows us to utilize continuous optimization techniques, and thus find a local optima.

2.2 The Graph Matching Problem

Consider two graphs, G_1 and G_2, with vertex sets $V_1, V_2 = \{1, 2, ..., n\}$ and corresponding adjacency matrices $A, B \in \mathbb{R}^{n \times n}$. The Graph Matching Problem (GMP) seeks to find a bijection $\phi : V_1 \to V_2$ such that the number of edge disagreements between G_1 and G_2 via ϕ is minimized. In matrix notation, the GMP is

$$\begin{aligned} &\min ||A - PBP^T||_F^2 \\ &\text{s.t. } P \epsilon \mathcal{P} \end{aligned} \tag{2.3}$$

where $||.||_F$ is the Frobenius norm. A special case of the GMP is known as a graph isomorphism, when there exists $P \in \mathcal{P}$ such that $A = PBP^T$. Expanding the objective function:

$$||A - PBP^T||_F^2 = trace\{(A - PBP^T)^T(A - PBP^T)\} = \\ trace(A^TA) + trace(B^TB) + 2 * trace(APB^TP^T) \tag{2.4}$$

Dropping constant terms, (2.4) is equivalent to

$$\begin{aligned} &\min \ -\text{trace}(APB^TP^T) \\ &\text{s.t.} \ \ P \epsilon \mathcal{P} \end{aligned} \tag{2.5}$$

We see that the objective function for the GMP is just the negation of the objective function for the QAP, and thus any algorithm that solves one can solve the other.

2.2.1 FAQ

The state-of-art FAQ algorithm of Vogelstein et. al, 2015, uses the Frank-Wolfe algorithm to find a doubly stochastic solution to (2.2), then uses the linear assignment problem to project this solution back onto the set of permutation matrices, thus approximately solving the QAP and GMP. In 2019, Fishkind et al. proposed modifications to FAQ to extend it's application to allow for seeds

(a known bijection subset) and graphs different sizes.

Algorithm 1: FAQ

Result: Find local optimum for the QAP

Inputs: Adjacency matrices $A, B \in \mathbb{R}^{n \times n}$

Initialize: $P^{(0)} \in \mathcal{D}$, barycenter unless otherwise specified **for** *i = 1, 2, 3, ... (and stopping criterion not met)* **do**

1. Compute $\nabla \mathrm{f}(\mathrm{P}^{(i)}) = AP^{(i)}B^T + A^T P^{(i)} B$
2. Compute $Q^{(i)} \in argmin \ \ trace(Q^T \nabla f(P^{(i)}))$ over $Q \in \mathcal{D}$ via Hungarian Algorithm.
3. Compute step size $\alpha^{(i)} \in argmin \ \ f(\alpha P^{(i)} + (1-\alpha)Q^{(i)})$, for $\alpha \in [0,1]$
4. Set $P^{(i+1)} = \alpha P^{(i)} + (1-\alpha)Q^{(i)}$

end

return $\hat{Q} \in argmax \ \ trace(Q^T \nabla f(P^{(final)}))$ over $Q \in \mathcal{P}$ via Hungarian algorithm.

Chapter 3

FAQ to GOAT

The primary computational bottleneck in FAQ is the linear assignment problem solved in step 2 (algorithm 1), with the most commonly used linear assignment algorithms (Hungarian and Jonker-Volgenant) having a time complexity of $O(n^3)$ (Jonker, Volgenant, 1987). Additionally, even if the adjacency matrix inputs are sparse, the gradient matrix calculated will in practice be dense, and thus sparse LAP solvers will not improve runtime.

Though it is known that the solution to maximizing $trace(Q^T \nabla f(P^{(i)}))$ over $Q \in \mathcal{D}$ can be chosen to be a permutation matrix (allowing for the use of LAP solvers), we argue that it should not always be selected to be a permutation matrix. This is due to the possibility that this maximization may have multiple solutions (this may also be referred to as a "tie"). Consider the following matrix

$$M = \begin{pmatrix} 40 & 50 & 60 & 65 \\ 30 & 38 & 46 & 48 \\ 25 & 33 & 41 & 43 \\ 39 & 45 & 51 & 59 \end{pmatrix}$$

Maximizing $trace(Q^T M)$ over $Q \in \mathcal{P}$ (the feasible region via the linear assignment problem), yields two optimal solutions:

$$P_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad and \quad P_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

each with objective function value 172. Linear Assignment algorithms in general settle these ties in a deterministic manner, thus making the final FAQ solution depen to the original bijection between A and B. In practice, we avoid such bias by randomly shuffling the nodes of B multiple times at a single intiliaization. However, such a method can be extremely computationally burdensome, especially when matching large graphs ($n > 10,000$).

Additionally, when such a tie is present, we have no reason to choose one solution over another. Indeed, it is easily shown that when multiple optimal solutions exist, all convex combinations of those solutions are also a solution.

Lemma 3.0.1. *Given matrix $M \in \mathbb{R}^{n \times n}$ with i possible $P_i \in argmax \ \ trace(Q^T M)$ over $Q \in \mathcal{P}$, then $\sum_{i=1}^{n} \lambda_i P_i \in argmax \ \ trace(Q^T M)$ over $Q \in \mathcal{D}$, such that $\sum_{i=1}^{n} \lambda_i = 1$ and $\lambda_i \in [0, 1]$.*

Proof. Consider $\forall \ \ P_i, \exists \ \ v \in \mathbb{R}^n$ such that $trace(P_i^T M) = v$.
From Birkhoff's Theorem, it's known that $\sum_{i=1}^{n} \lambda_i P_i \in \mathcal{D}$.
$trace(\sum_{i=1}^{n} \lambda_i P_i M) = \sum_{i=1}^{n} trace(\lambda_i P_i M) = \sum_{i=1}^{n} trace(\lambda_i P_i M) = \sum_{i=1}^{n} \lambda_i trace(P_i M) =$

$\sum_{i=1}^{n} \lambda_i v = v$ □

We thus seek a method of solving step 2 that is deterministic and independent of the initial shuffle on our input matrices, while also balancing the possible optimal permutation matrix solutions into a single optimal doubly stochastic matrix solution.

3.1 Lightspeed Optimal Transport

3.1.1 Transportation and Sinkhorn Distances

The optimal transport problem is a fundamental probability and optimization problem, in which the transportation of object μ to v is minimized by some cost. More formally, consider the transportation polytope

$$U(r, c) = \{P \in \mathbb{R}^{n \times n} | P\mathbf{1}_n = r, P^T\mathbf{1}_n = c\} \tag{3.1}$$

where $U(r, c) \in \mathbb{R}^{n \times n}$, non-negative, with row and column sums equal to r and c, respectively, and $\mathbf{1}_n$ is the n-dimensional vector of ones. The optimal transport problem is thus defined as

$$\begin{aligned} &\min \ \langle P, M \rangle \\ &\text{s.t.} \ \ P \in U(r, c) \end{aligned} \tag{3.2}$$

where $M \in \mathbb{R}^{n \times n}$ is the cost matrix. Cuturi (2013) proposed to modify optimal transport through the addition of a regularizing entropic penalty, $h(P)$

resulting in the *Sinkhorn distance* formulation

$$\begin{aligned} &\min \ \langle P, M \rangle - \frac{1}{\lambda} h(P) \\ &\text{s.t.} \ \ P \in U(r, c) \end{aligned} \tag{3.3}$$

where $\lambda \in [0, \infty]$, with the Sinkhorn and transportation distances equivalent for λ suitably large; that is, as λ approaches ∞, the Sinkhorn distance solution approaches the optimal transport solution. Cuturi showed that Sinkhorn distances could be solved using Sinkhorn-Knopp's fixed point iteration algorithm (citation here), on $e^{-\lambda M}$, demonstrating that the method performed very well in practice, and was computationally fast.

3.1.2 Doubly Stochastic Optimal Transport

Setting $r, c = \mathbf{1}_n$, the transportation polytope is equivalent to the Birkhoff polytope, also known as the set of doubly stochastic matrices ($U(\mathbf{1}_n, \mathbf{1}_n) = \mathcal{D}$). We consider this to be a family of optimal transport, and refer to it as the *doubly stochastic optimal transport problem*. Additionally, since $\langle P, M \rangle = trace(P^T M)$, the doubly stochastic optimal transport problem can be written as:

$$\begin{aligned} &\min \ trace(P^T M) \\ &\text{s.t.} \ \ P \in \mathcal{D} \end{aligned} \tag{3.4}$$

which is precisely equivalent to the relaxed linear assignment problem (rLAP). Thus, we may use Sinkhorn distances to solve the rLAP. We define the rLAP algorithm inspired by Cuturi as *Lightspeed Optimal Transport* (LOT) in algorithm 2. To solve the maximization aLAP problem, simply negate M. In practice, we

choose $\lambda \geq 100$.

Algorithm 2: LOT

Result: Find doubly stochastic solution to rLAP
Inputs: Cost matrix $M \in \mathbb{R}^{n \times n}$, $\lambda \in \mathbb{R}$

1. Compute $K \leftarrow e^{-\lambda M}$
2. Compute $Q \leftarrow Sinkhorn(K)$

return Q

To demonstrate LOT's effectiveness, we independently realize 100 cost matrices $M \in \mathbb{R}^{n \times n}$ for $n = 250, 500, ..., 3000$, where each entry $M_{i,j} \ \ \forall i, j \in n$ is sampled randomly from the Uniform(100,150) distribution.

In Figure 3.1, we observe that using LOT rather than traditional LAP algorithms causes a substantial speed increase, with little loss in performance, with percent difference in objective function value less than 1%.

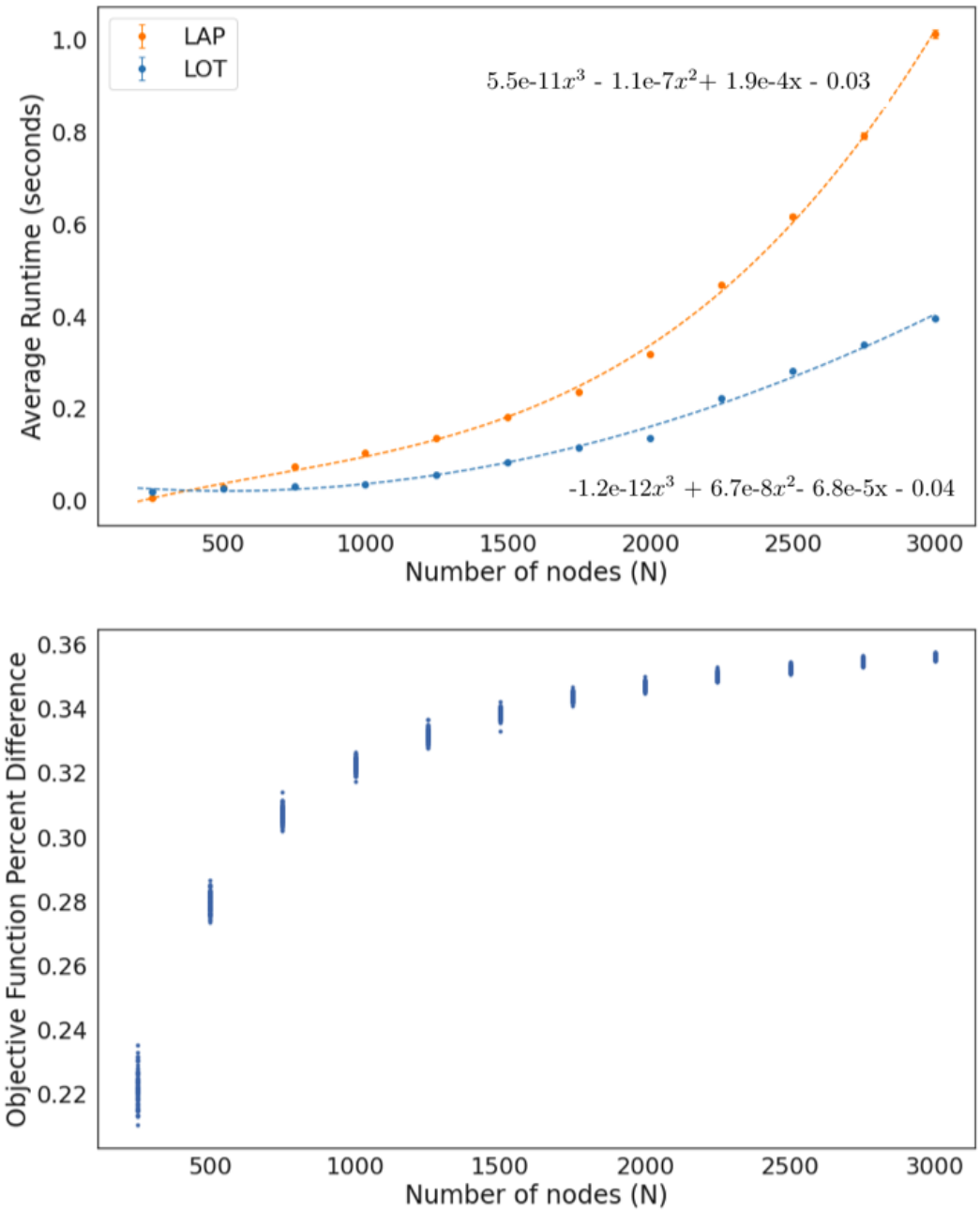


Figure 3.1: Running time and performance of LAP and LOT as a function of number of nodes, n. Cost matrix sampled from a Uniform(100, 150) distribution, with 100 simulations per n. Performance defined as relative accuracy, $\frac{OFV_{LAP}-OFV_{LOT}}{OFV_{LAP}}$, with each dot representing a single simulation.

Chapter 4

GOAT

In this section, we introduce the **GOAT** algorithm, a modification of the state-of-the-art FAQ algorithm.

Algorithm 3: GOAT

Result: Find local optimum for Graph Matching Problem
Inputs: Graphs G_1, G_2 with vertex sets $V_1, V_2 = \{1, 2, ..., n\}$, and associated adjacency matrices $A, B \in \mathbb{R}^{n \times n}$
Initialize: $P^{(0)} \in \mathcal{D}$, barycenter unless otherwise specified
for *i = 1, 2, 3, ... (and stopping criterion not met)* **do**

1. Compute $\nabla \mathrm{f}(\mathrm{P}^{(i)}) = AP^{(i)}B^T + A^TP^{(i)}B$
2. Compute $Q^{(i)} \in argmax \ \ trace(Q^T \nabla f(P^{(i)}))$ over $Q \in \mathcal{D}$ via Lightspeed Optimal Transport.
3. Compute step size $\alpha^{(i)} \in argmax \ \ f(\alpha P^{(i)} + (1-\alpha)Q^{(i)})$, for $\alpha \in [0, 1]$
4. Set $P^{(i+1)} = \alpha P^{(i)} + (1-\alpha)Q^{(i)}$

end
return $\hat{Q} \in argmax \ \ trace(Q^T \nabla f(P^{(i)}))$ over $Q \in \mathcal{P}$ via Hungarian algorithm.

Replacing the bottleneck LAP step with the fast and accurate LOT algorithm makes GOAT faster on larger graphs and adds robustness when solving

graph matching problems when two graphs are not isomorphic. Rather than tie breaking like LAP solvers, LOT distributes weight across the similar nodes in the doubly stochastic step direction matrix, Q.

When initializing GOAT, we typically choose the doubly stochastic barycenter, $J = \mathbf{1}_n * \mathbf{1}_n^T / n$ as the initialization, though any doubly stochastic matrix is feasible. If the graphs are sufficiently small, we can also use several random initializations to maximize performance. Specifically, we independently run GOAT for many $P^{(0)} = \frac{1}{2}(J + K)$, where K is a random doubly stochastic matrix via Sinkhorn-Knopp, and choose the permutation with the best associated objective function value.

In step 3, α can be computed exactly. Consider $g(\alpha) = f(\alpha P^{(i)} + (1 - \alpha)Q^{(i)})$. Since g is quadratic, it can be represented as $g(\alpha) = b\alpha^2 + c\alpha + d$ $(b, c, d \in \mathbb{R})$. To find the max of this value we set it's derivative, $g'(\alpha) = 2 * b\alpha + c$, to zero and solve for alpha, yielding $\hat{\alpha} = -c/2b$. Let $R = P - Q$.

$$\begin{aligned} g(\alpha) &= f(\alpha P^{(i)} + (1-\alpha)Q^{(i)}) = f(\alpha R + Q) \\ &= trace(A(\alpha R + Q)B^T(\alpha R + Q)^T) \qquad (4.1) \\ &= \alpha(trace(ARB^TQ^T) + trace(AQB^TR^T)) + \alpha^2 trace(A = RB^TR^T) \end{aligned}$$

Then:

$b = trace(ARB^TR^T)$

$c = trace(ARB^TQ^T) + trace(AQB^TR^T)$

For the final step of the algorithm, we must still use a LAP solving algorithm to project the doubly stochastic P^{final} onto the set of permutation matrices.

Chapter 5

Software

All algorithms mentioned previously, including but not limited to FAQ, SGM, GOAT, LOT, and the experiments shown later, are implemented in Python, an interpreted, general purpose programming language, and are available at https://github.com/neurodata/gmot.

Additionally, the algorithms FAQ and SGM, are available as a function (implemented by the author) in the Python open-source package **SciPy**. FAQ and SGM have the following signature.

```
scipy.optimize.quadratic_assignment(A, B, method='faq')
```

where A and B are the adjacency matrices. Additionally, a dictionary of options can be passed into the function to allow the user to choose whether they would like to solve the QAP or GMP, or if they would like to include seeded vertices. More details on the other options the function can accept can be found in the documentation.

The usage of the function is shown below. In the example, we sample two random 15 node adjacency matrices, using FAQ to solve for the minimum

objective function value.

```
>>> from numpy.random import default_rng
>>>
>>> rng = default_rng()
>>> n = 15
>>> A = rng.random((n, n))
>>> B = rng.random((n, n))
>>>
>>> res = quadratic_assignment(A, B)  # FAQ is default method
>>> print(res.fun)
46.871483385480545  # may vary

>>> options = {"P0": "randomized"}  # randomized initialization
>>> res = quadratic_assignment(A, B, options=options)
>>> print(res.fun)
47.224831071310625 # may vary
```

The resulting optimization object from running **quadratic_assignment** has attributes *fun* (objective function after convergence), *col_ind* (permutation/bijective after convergence), and *nit* (number of iterations to converge).

FAQ and SGM are also implemented in the GraphMatch object in the open-source graph statistics package **microsoft/graspologic**.

Additionally, the Jonker-Volgenant LAP algorithm is also implemented in **SciPy**, with the following signature.

```
scipy.optimize.linear_sum_assignment(cost_matrix,
                                     maximize=False)
```

Chapter 6

Results

We explore the effectiveness of GOAT on simulated and real data examples, measured through matching ratio (the fraction of nodes that are correctly aligned), objective function value, and runtime. Since GOAT is a modification of FAQ, we demonstrate the advantages of GOAT to FAQ in each of our experiments.

6.0.1 Simulation Setting

In our simulations, we sample graph pairs G_1, G_2 from a ρ-correlated Stochastic Block Model (SBM). The ρ-SBM model is given:

1. Number of nodes per block, $n \in \mathbb{R}^k$, where $k \in \mathbb{Z}_{>0}$ is the number of blocks.

2. Edge probability matrix $X \in [0,1]^{k \times k}$, where $X_{i,j}$ represents the probability of an edge between nodes in community $[i, j]$.

For this model, $\rho = 0$ implies that the graph pairs are independent, and $\rho = 1$ implies that the graph are isomorphic. The SBM model maintains a

one-to-one node correspondence across graph pairs, while also incorporating stochasticity.

Additionally, the ρ-correlated Erdos-Reyni (ER) model can be considered a special case of ρ-SBM, in which $k = 1$.

6.0.2 Space and Time Complexity

As noted earlier, even if the adjacency matrix inputs for GOAT are sparse, the gradient matrix computed will likely be dense. Thus, GOAT and FAQ share a space complexity of $O(n^2)$, the space required to store $\nabla f(P)$.

In Fig 6.1, we demonstrate the computational advantages of GOAT over FAQ through it's run-time, especially with larger n. Since a LAP solver is still required in the final step of the algorithm to project P^{final} onto the set of permutation matrices, as well as the matrix multiplication required, GOAT has a time complexity of $O(n^3)$, equivalent to that of FAQ. However, in Fig 6.1, we observe that GOAT leading constant is an order of magnitude smaller than that of FAQ.

Additionally, GOAT far outperforms FAQ in terms of its performance, consistently recovering the exact match between graph pairs for each n. It's important to note, however, that FAQ appears to have a faster runtime for smaller n, specifically $n < 200$. Nonetheless, GOAT's performance scales very well, with consistently exact match ratios as n increases.

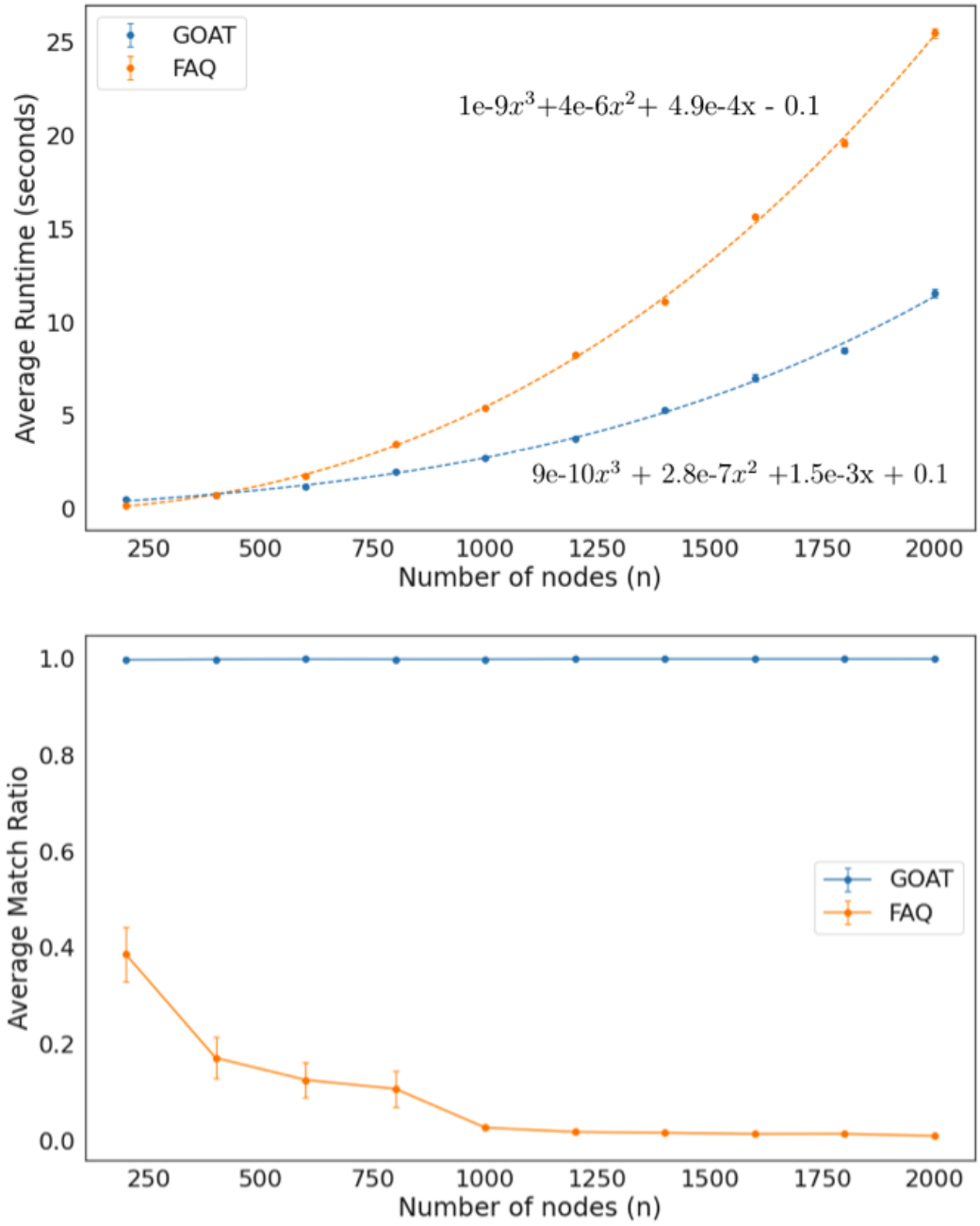


Figure 6.1: Average running time and match ratio $\pm$ 2 s.e. of FAQ and GOAT as a function of number of nodes, n. Data sampled from a ρ-correlated Erdos-Reyni model, with $\rho = \frac{log(n)}{n}$, with 50 simulations per n.

6.0.3 Simulation Results

Our first simulation result is focused on assessing GOAT's performance in recovering the underlying node correspondence between two graphs. To model a setting in which this correspondence exists, we sample graph pairs G_1, G_2 from a ρ-correlated SBM.

In our first experiment, we independently sample 100 ρ-SBM graph pairs for each value of $\rho = \{0.5, 0.6, \ldots, 1.0\}$ on 150 nodes where $k = 3$, and

$$X = \begin{pmatrix} 0.2 & 0.01 & 0.01 \\ 0.01 & 0.1 & 0.01 \\ 0.01 & 0.01 & 0.2 \end{pmatrix}$$

with each block containing an equal number of nodes. We additionally sample 25 independent ρ-SBM graph pairs for each value of $\rho = \{0.8, 0.85, \ldots, 1.0\}$ on 1500 nodes, with the same k and X above. For each pair of graphs, we run both FAQ and GOAT and measure the match ratio, defined as fraction of correctly aligned nodes to total nodes. For each ρ value, we plot the average match ratio over the graph pairs, along with twice the standard error (Fig 6.2).

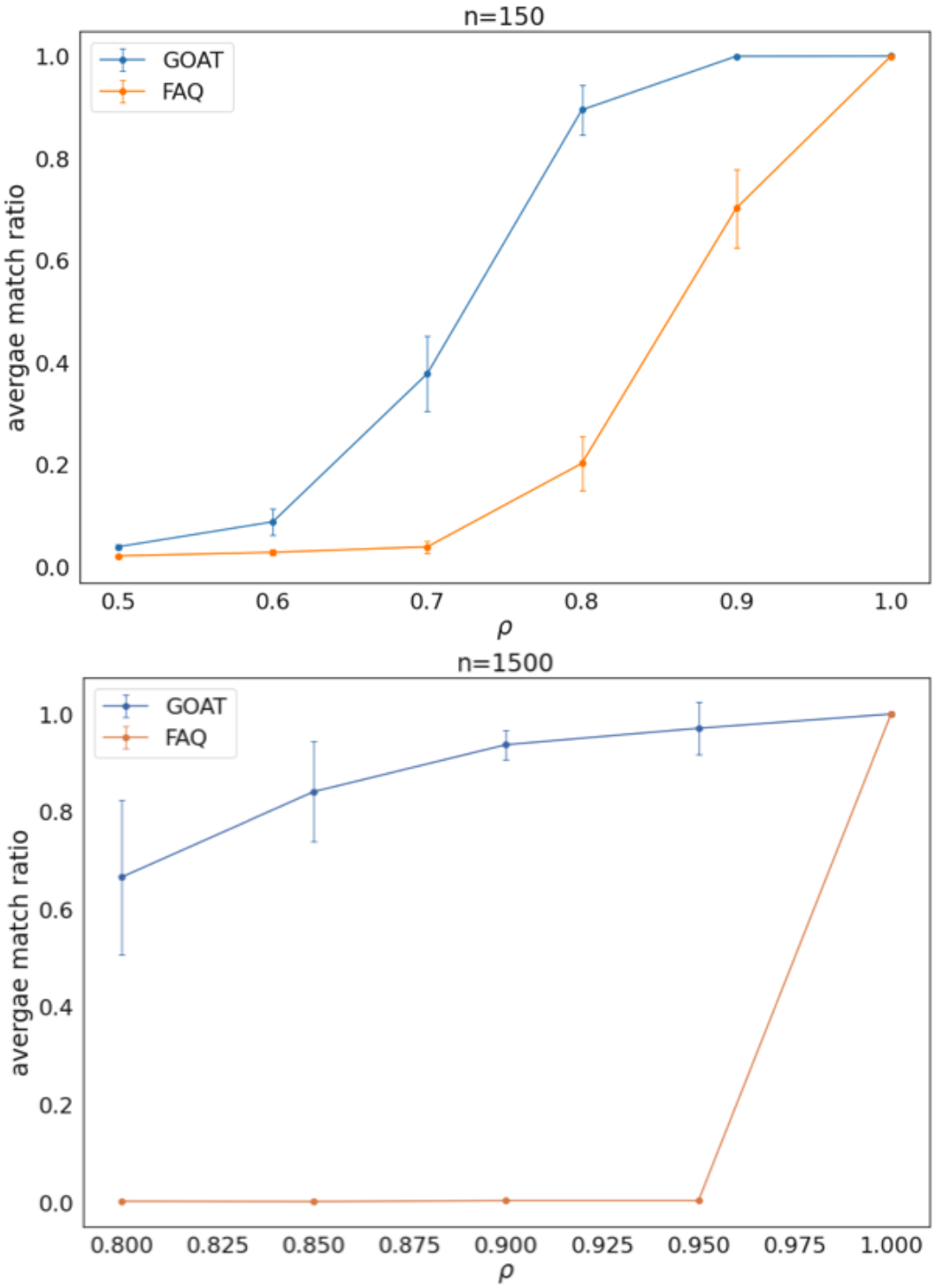


Figure 6.2: Average match ratio $\pm$ 2 s.e. as a function of correlation values ρ in ρ-SBM simulations on $n = 150, 1500$ nodes.

Across both experiments, we note that GOAT consistently reports a matching accuracy that is greater than or equal to that of FAQ, with the difference increasing as ρ decreases. Additionally, we highlight that GOAT often far outperforms FAQ, with instances in which GOAT consistently reports match ratios close to 1, while FAQ reports ratios close to 0. As expected, GOAT provides robustness to the graph matching results as randomness is added to the network. It is important to note that in real-data settings, networks are often large and highly correlated, but rarely isomorphic. Indeed, when n=1500, the performance gap between FAQ and GOAT is even more noticeable, and when $\rho = 0.95$, GOAT consistently recovers the exact alignment, while FAQ reports an average match ratio < 0.1.

In our next experiment, we investigate GOAT's effectiveness in solving the seeded graph matching problem. Applying Fishkind, et. al's modification to both FAQ and GOAT, we run the following experiment, inspired by Figure 2 in Fishkind, 2019. We independently sample 100 ρ-SBM graph pairs for each value of $\rho = \{0.3, 0.6, 0.9\}$ on 300 nodes where $k = 3$, and

$$X = \begin{pmatrix} 0.7 & 0.3 & 0.4 \\ 0.3 & 0.7 & 0.3 \\ 0.4 & 0.3 & 0.7 \end{pmatrix}$$

with each block containing an equal number of nodes. For each rho value, we plot the average match ratio (over the 100 independent realizations) as a function of the number of seeds, m.

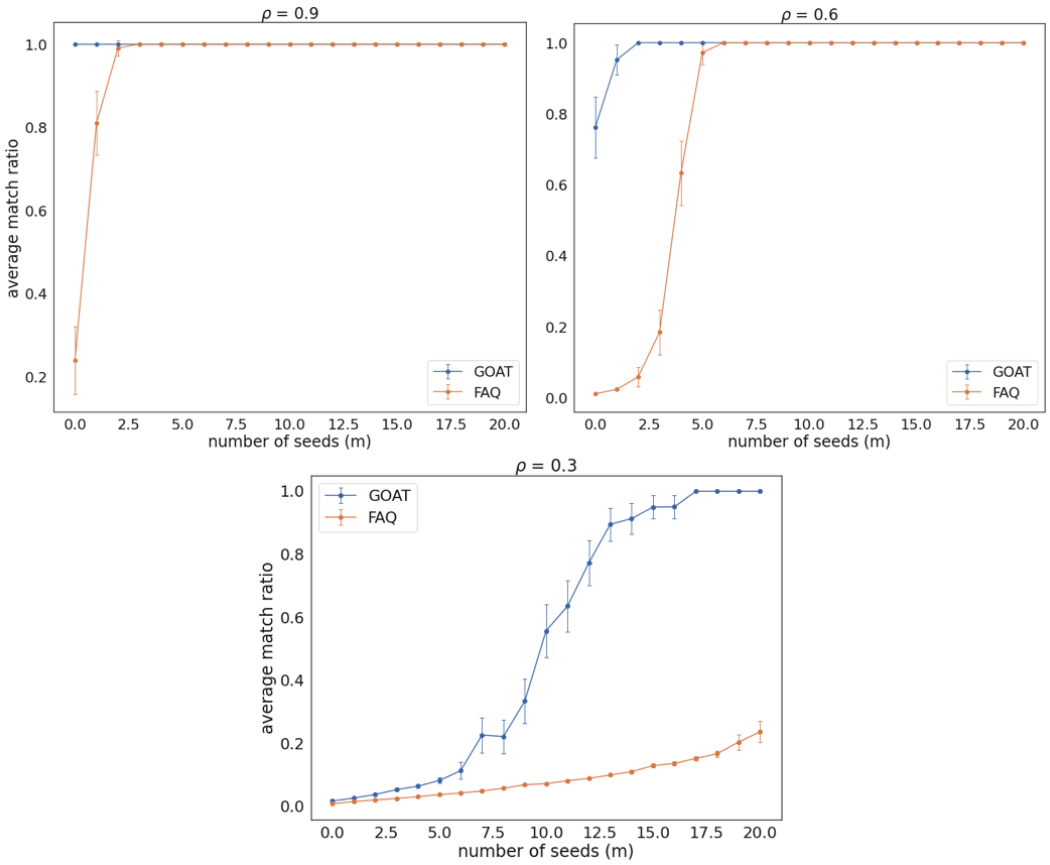


Figure 6.3: Average match ratio $\pm$ 2 s.e. as a function of number of seeds m for correlation values $\rho = 0.3, 0.6, 0.9$ in ρ-SBM simulations on $n = 300$ nodes.

In Fig 6.3 we observe that, with all ρ experiments, GOAT requires fewer seeded vertices than FAQ to converge to the exact matching. Additionally, when $\rho = 0.3$ GOAT converges to finding the exact matching, while FAQ does not, with FAQ's matching accuracy less than 0.2 compared to GOAT's accuracy of 1.0.

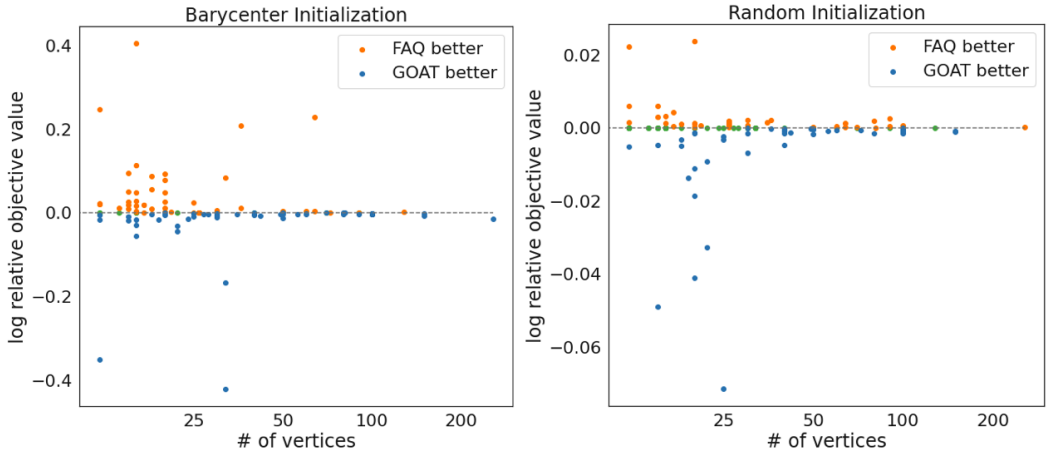
6.0.4 QAPLIB Benchmark

In order to benchmark GOAT's performance against FAQ's, we evaluate the algorithm's performance on the QAPLIB, a standard library of 137 quadratic assignment problems (Burkard, 1997). Performance is measured by minimizing the objective function $f(P) = trace(APB^TP^T)$. In Figure 6.4, we plot the log (base 10) relative accuracy $\frac{f_{GOAT}}{f_{FAQ}}$ for each of the 137 QAPLIB instances, with two initialization schemes:

1. Random initialization: the minimum objective function value over 100 initializations at $P = \frac{1}{2}(J + K)$, where J is the doubly stochastic barycenter, and K is a random doubly stochastic matrix.

2. Barycenter initialization: a single initialization.

Note that a random shuffle on B is performed at each initialization prior to running the algorithms, and random shuffles and initializations are consistent across GOAT and FAQ (the same are used for both methods).



Method	% better
GOAT	47.5
FAQ	41.8
Tie	10.7

Method	% better
GOAT	34.4
FAQ	33.6
Tie	32

Figure 6.4: Relative accuracy between FAQ and GOAT, defined as y=log($\frac{f_{GOAT}}{f_{FAQ}}$). Performance is compared using the minimum objective function value over 100 random initializations, and the objective function value of a barycenter initialization with one random shuffle. Initializations and shuffles are the same across FAQ and GOAT.

We note that GOAT performs better on a marginally larger portion of the QAPLIB problems. Using the Mann-Whitney U test, due to it's robustness to ties, we observe p-values of 0.50 and 0.49 for the random and barycenter initializations, respectively, failing to reject the null hypothesis that the probability of GOAT performing better than FAQ is equal to the probability of FAQ performing better than GOAT. This result demonstrates that replacing the exact LAP solver with an approximate algorithm causes no significant loss in performance.

Chapter 7

Discussion and Conclusion

In this work, we have summarized the existing methodology in continuous optimization for solving the graph matching and quadratic assignment problems, and introduced a modification to the state-of-art FAQ algorithm, making it faster on larger graphs, and improving accuracy on simulation benchmarks used in literature.

In our simulated experiments, we demonstrated that GOAT was faster than FAQ on larger graphs, and often far outperformed FAQ when finding accurate bijections across graph pairs. Additionally, we showed that when graph pairs were not isomorphic, as is often the case in real data, GOAT was again better than FAQ at finding accurate bijections across graph pairs. Further, using the QAPLIB benchmarks, which has smaller graphs than those used in simulations, we demonstrated that GOAT still performs as well as FAQ.

In the future, we would like to test GOAT's performance on real-world, large graph data, investigating how GOAT performs on graphs with more than 10,000 nodes. Additionally, we would like to explore other methods

of improving the runtime and accuracy of graph matching and quadratic assignment algorithms.

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Curriculum Vitae

Ali Saad-Eldin was born on Long Island, NY and grew up in Smithtown, NY. He attended Johns Hopkins University where he studied Biomedical Engineering and minored in Applied Mathematics and Statistics, completing his Bachelor of Science in May 2020. He subsequently earned his Master s degree from Johns Hopkins University in May 2021, studying Biomedical Engineering with a focus in Biomedical Data Science.